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Dynamics of a network of hydrogen bonds upon water electrocrystallization

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Abstract

Computer simulation is employed to study the dynamics of a network of hydrogen bonds and the structural properties of water placed between graphene layers. The presence of the graphene walls has been shown to substantially affect the water phase diagram. Glass transition processes are observed in the system, and liquid water completely passes to an amorphous state. Moreover, it has been established that the imposition of an external electric field with strength $E \geq 0.5$ V/Å on the system subjected to increased pressure results in structural ordering of water. It has been found that water located between graphene layers is transformed into Ic cubic ice. The electrocrystallization of water has been shown to substantially change the dynamics of the network of hydrogen bonds.

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